研究ノート

Monte Carlo Simulation of Phase Transitions

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In the Monte Carlo simulation of phase transition, a simple heat bath method is applied to the classical Heisenberg model in two dimensions. It reproduces the correlation length predicted by the Monte Carlo renormalization group and also computed in the non-linear σ model.

1. Introduction and conclusions

The qualitative agreement of QCD (Quantum chromodynamics) perturbative calculations with experiment is an indication that QCD, a SU(n) gauge theory, is the correct dynamical theory of quarks. The Monte Carlo computor simulation has been applied to a formulation of QCD on a discrete space-time lattice in order to bridge a gap between the asymptotic freedom at short range of the interaction and the confinement at long range. It is supposed [1] that, in the lattice model, the O(3) spin model in two dimensions has a series of properties which are analogous to those of gauge theories with the group SU(3) in four dimensional space.

The aim of this paper is two-fold: the one is to apply a simplified version of the heat bath method of the Monte Carlo optimization to the classical O(3) spin model (Heisenberg model) in two dimensions. The other is to obtain technical data of the simulation on a MELCOM 70 MODEL 40, a computor of small capacity with a 16-bit central processing unit, for the convenience of further studies of lattice models.

As conclusions, our heat bath algorithm works well in reproducing the predictions [2, 3] on the spin correlation length of the nonlinear σ model and of the Monte Carlo renormalization group. The method has made computation time considerably short. But the reduction would not be sufficient in its application to gauge models, if we use the FORTRAN language. The whole random rearrangement step should be written in the assembly language, while we wrote only the generator of quasi-random numbers in it in this work.

The evidence for a transition of the Kosterlitz-Thouless type [4] is quite strong in the O(2) spin models of two dimensions [5]. It has commonly*) been supposed that the two-dimensional O(3) spin model with nearest-neighbour feromagnetic interactions do not undergo phase transition [2, 7, 8]. For O(n) ($n \geqq 3$), transitions involving a spontaneous order are certainly excluded by the Mermin-Wagner theorem [9]. A possibility of topological phase transition in the O(3) model has been examined with the Monte Carlo technique [10, 11].+) Additional supports for the premise that no phase transition occurs in the model come from renormalization group arguments [13] and from the one-loop approximation in the instanton picture of the non-linear σ model [14, 15]. As far as the author knows, we have not a completely analytic proof of the non-existence of phase transition in the classical Heisenberg model of two dimensions. The hope is that the global analysis [16] can give a final resolution on this problem.

Recently, the role of monopoles has drawn our attention in the confinement of quarks. There is a controversy on the existence of phase transition [17] in the $O(3)/Z_2$ model.

This paper will be organized as follows. Section 2 deals with the techniques of the Monte Carlo simulation. Results will be presented in section 3. The bulk of remainder of this section is devoted

*) The existence of a phase transition was conjectured in ref. [6].

+) Similar studies were made also in the gauge models [12].

to explanation of our models.

The lattice spin model is defined by the following action;

$$S=-\sum_{<i,j>} Js_i s_j-\sum_j s_j H \qquad (1.1)$$

where J is the coupling constant and H is uniform magnetic field. The spin variable s_i on the lattice point i is a real unit 3-vector for the classical Heisenberg model and ± 1 for the Ising model. The unit of temperature is chosen so that the Boltzmann constant $k=1$ and the critical temperature is normalized to be one in the Ising model. This is to take $J=-\ell n(\sqrt{2}-1)/2$ by Onsager's solution [18]. For the Heisenberg model $J=1$. Throughout this paper, we consider only nearest-neighbour seits$<i,j>$on a square lattice and the case of zero magnetic field: $H=0$. The periodic boundary condition will be imposed on s_i, that is, the lattice is on a torus.

2. Algorithm

A. Generation of quasi-random numbers

The multicative congruent method is the simplest one of obtaining a sequence of quasi-random numbers. The sequence is defined by the linear recurrence relation

$$x_{n+1}=\lambda x_n \bmod P \ (n=0,\ 1,\dots), \qquad (2.1)$$

where the factor λ and the modulus P are integers and the normalized numbers

$$y_n=x_n/P \ (n=0,\ 1,\dots) \qquad (2.2)$$

are uniform deviates in the interval $[0,1]$. For the Ising model, $\lambda=899$ and $P=2^{15}$, where the values are employed in Numerical Subroutine Package (NSP) of MELCOM 70, and $\lambda=5^{11}$ and $P=2^{30}$ [19] for the Heisenberg model.

It is well known that the maximum period of the sequence of quasi-random numbers is 2^{m-2}, when the modulus $P=2^m$ [19]. In our generator, the odd initial value x_0 is replaced five times every two-thirds of the maximum period.

B. The updating procedure

The heat bath method [20, 21] of the Monte Carlo simulation consists of successively touching a heat bath to each spin of the lattice while holding fixed the spins at the remaining lattice points. Repeating this procedure eventually produces a sequence of states which simulates an ensemble of such systems in thermal equilibrium. Beginning in some initial configuration of the spins, we pass through the entire lattice varying one spin at a time, whose lattice point is chosen with two random numbers.

In this paper, we compare the following two ways of determining a new spin at each spin's turn.

(H1) [21] This choice is made randomly from the entire group with weighting proportional to the Boltzmann factor

$$B(s)=\exp\ (\sum_i Js\cdot s_i/kT), \tag{3.5}$$

where s_i's are the nearest-neighbour spins of the current spin s and T is temperature. All other spins except the current spin are fixed with their previous values. The old values for the current spin plays no direct role in this procedure. We consider a unit sphere on which the tip of the spin moves, and approximate it with a polygon which has 1058 facets; the maximum semi-circle is divided into 24 sectors. Such an approximation is also made in the gauge models [22].

(H2) Another way of the choice is a simplification of the updating procedure in ref. [20]. The probability of choosing a new spin determined randomly proportional to $B(s)$ in eq. (3.5). We compare the probabilities for the new value and the old value of the current spin. If a random number uniform in [0, 1] falls on the interval between naught and the normalized probability for a new spin, we take the new value of the spin. Otherwise, the spin is fixed with the old value.

In what follows, an iteration is defined as the total application of the above algorithm to $N\times N$ spins chosen randomly, where the number N is the lattice size.

The heat bath method would be characterized as a rather shortsighted search strategy; each small step is concerned with its local optimizationwithout knowledge of the need of the whole system further down to the minimum of the free energy. We must compare Monte Carlo results, starting with different initial configurations of spins.

The Metropolis algorithm [23] for Monte Carlo optimization has been widely applied in order to avoid getting stuck at metastable local optima in search for the equilibrium configuration of spins. However, this method needs an artificial parameter, maximum allowed displacement from the old value of the spins. The heat bath technique (H2) do not involve any additional parameter.

3. Results

A. the Ising model

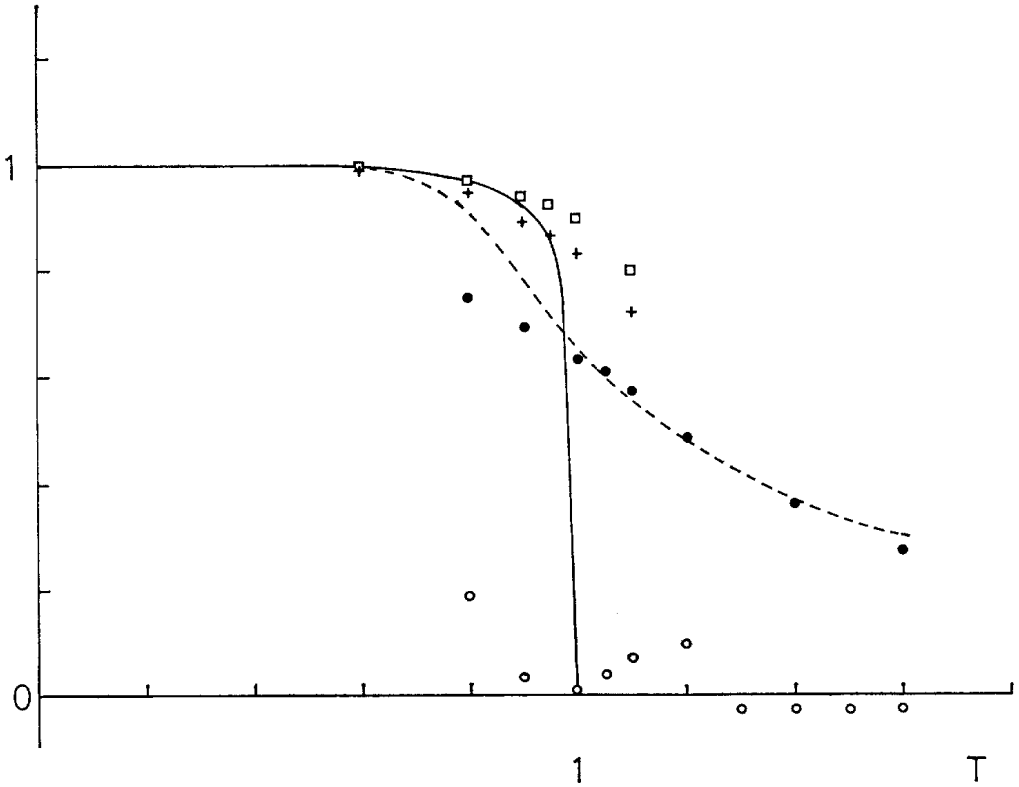

Fig. 1 The equilibrium values of polarization (□, ○) and of nearest-neighbour correlation (+, ●) in the Ising model on a 31×31 lattice. We make a comparison of them with the exact values varying with temperature. The crosses and the open squares correspond to ordered start. The open and closed circles represent the values with random start.

In figure 1, we compare the Monte Carlo results with the exact magnetization and nearest-neighbour correlation [24]. A phase transition is found as expected by the rigorous proof. An iteration by the method (H1) takes about 30 seconds including printing time.

B. the classical Heisenberg model

The heat bath method (H1) requires about 3 hours for an iteration on a 113×113 lattice. This computation time is too long to perform our whole calculation, so that we employ the method (H2), by which an iteration takes about 40 seconds on a 70×70 lattice.

Figure 2 shows the average energy E per link plotted against temperature. It is readily seen that there is no evidence for any phase transition. The specific heat is the gradient of E in fig. 2. It would show a broad peak in the cross-over region from low temperatures to high ones, however, this peak would be finite, supporting the absence of phase transition. The values obtained with the Metropolis technique [22] are naturally lower than our values.

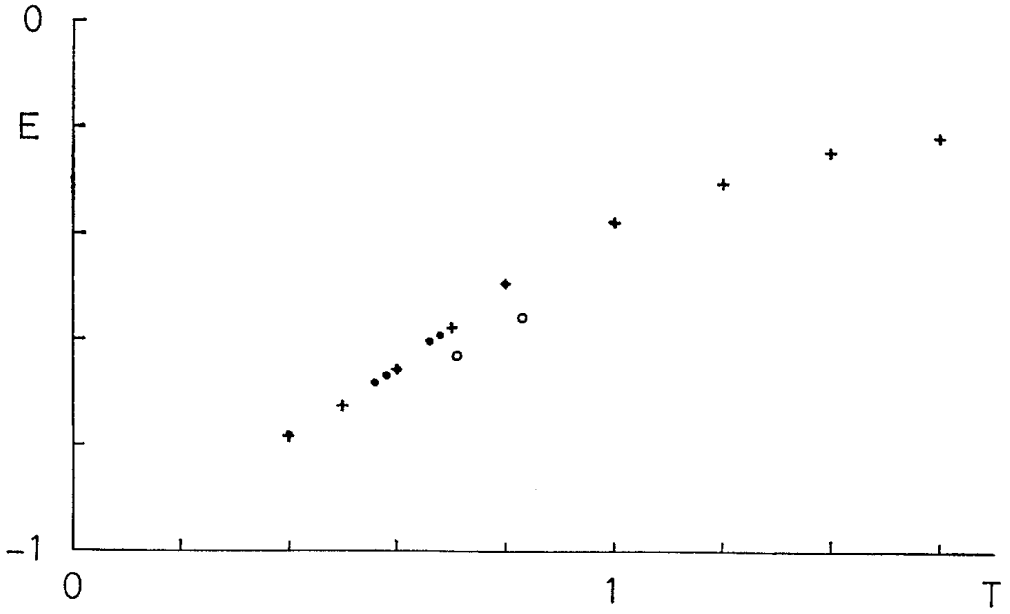

Fig. 2 The average energy per link for the classical Heisenberg model on a 70×70 lattice. Throughout this paper, the closed circle and the cross represent values computed with random start and ordered start, respectively. The values calculated with the Metropolis technique [11] are shown with open circles.

Figure 3 displays average two-spin correlation versus their lattice distance. The statistical errors have been calculated for 10 samples of successive 30 iterations. At low temperatures, we find discrepancy out of the statistical errors between the correlations computed with ordered start and those with random start at large distance. This is due to the fact that the recurrence "time" of correlation fluctuation is more than 30 iterations.

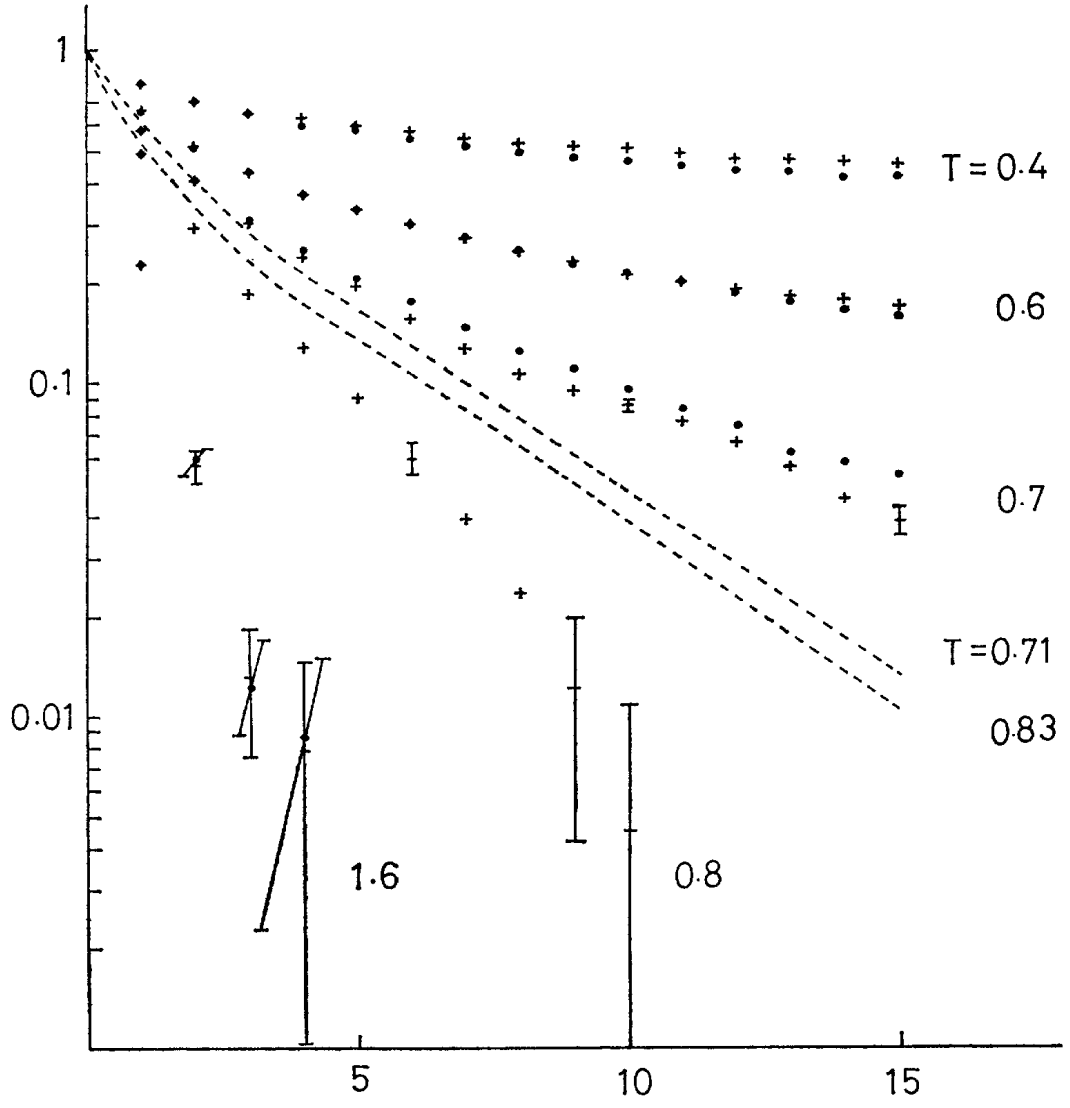

Fig. 3 The correlation functions n a logarithmic scale, which are plotted against lattice distance. Only the typical statistical errors are given. The dashed curves represent the results [11] by the Metropolis method.

The large statistical errors for the mean values under 0.01 would come from the finite size of the lattice*): $1/\sqrt{(70\times 70)} = 0.014$.

It can be seen from fig. 3 that the heat bath method (H2) brings out a rapid change of the correlation length in the cross-over region $T=0.6\sim 0.8$ as compared to the Metropolis method. At present, we do not know why the tail of the spin correlation at large distances is so sensitive to the computation methods.

The correlation length ξ was calculated [3] in the one loop approximation of the instanton approach [14] in the non-linear σ model:

$$\xi = \frac{\exp(1-\pi/2)}{32\sqrt{2}} \exp(2\pi/T) \left(\frac{T}{2\pi}\right) \tag{4.1}$$

This is the low-temperature result. The Monte Carlo renormalization group method [2] gives a similar form for ξ:

$$\xi = C \left(\frac{1}{1+2\pi/T}\right) \exp(2\pi/T), \tag{4.2}$$

where C is around 0.010 [2] or 0.0085 ± 0.0003 [26]. It can be seen from fig. 4 that our Monte Carlo result is in a good agreement with eqs. (4.1) and (4.2), but the agreement with the high-temperature expansion [2] is not so good. It should be noted that there are some ways of extracting the correlation length from the spin correlation functions. We determine ξ as a logarithmic slope around the value of ξ.

Figure 5 illustrates the spin correlation at the distance of 20 lattice spacings versus almost every 1000 iterations. The value with ordered start approached to the equilibrium value with random start at the 6000th iteration, however, it showed again a power-law correlation after more 1000 iterations as depicted in

*Some efficient method has been developed order to overcome this difficulty [25].

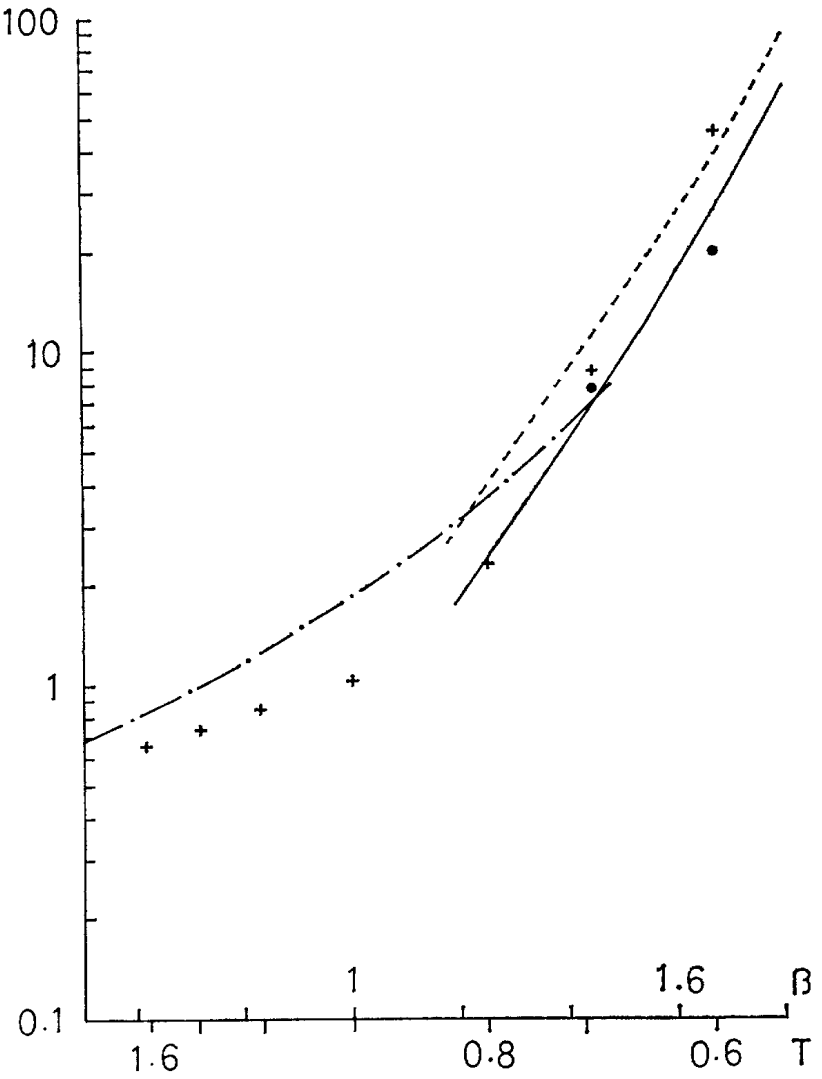

Fig. 4 The correlation length plotted versus the inverse temperature β. The solid curve and the dashed curve are the low-temperature approximants given by eqs. (4.1) and (4.2), respectively. The dashed and dotted curve represents the high-temperature expansion.

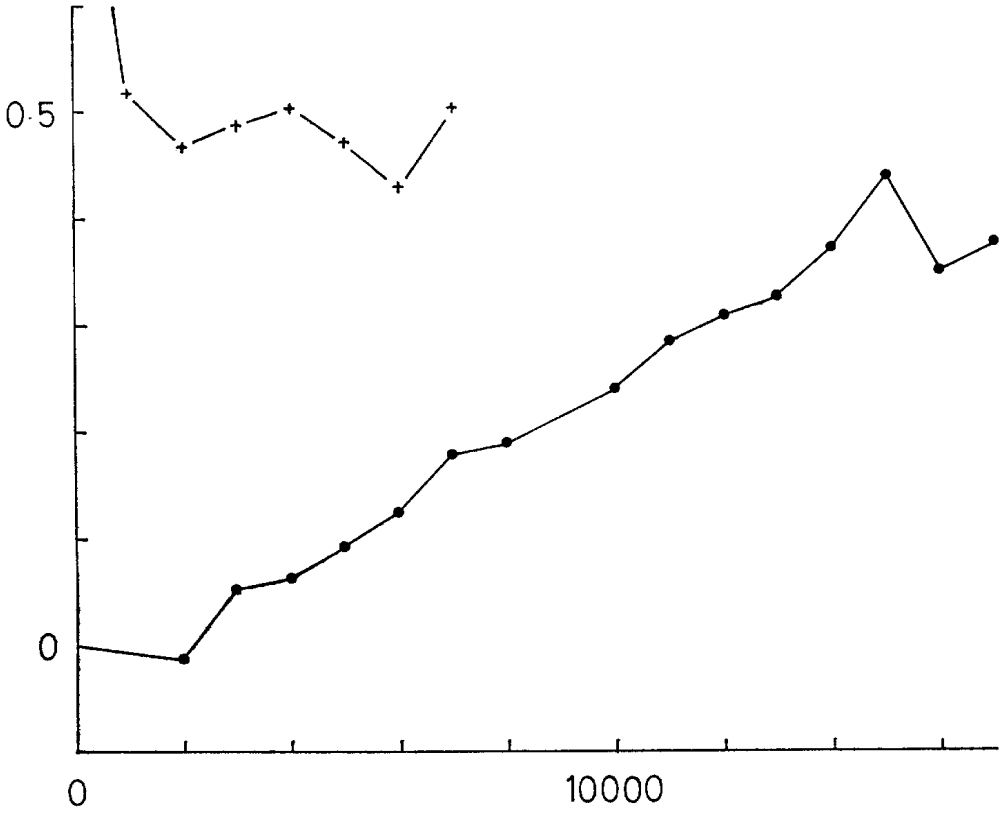

Fig. 5 At $T=0.4$, the correlation between two spins at the distance of 20 lattice spacings approaches the value of thermal equilibrium from an ordered state or from a random state with increasing number of the iterations.

fig. 6. This implies that the heat bath optimization can hardly gain access to the ground state at very low temperature of such a "frustrated" system with the expected degeneracy [11] as the two-dimensional O(3) spin model.

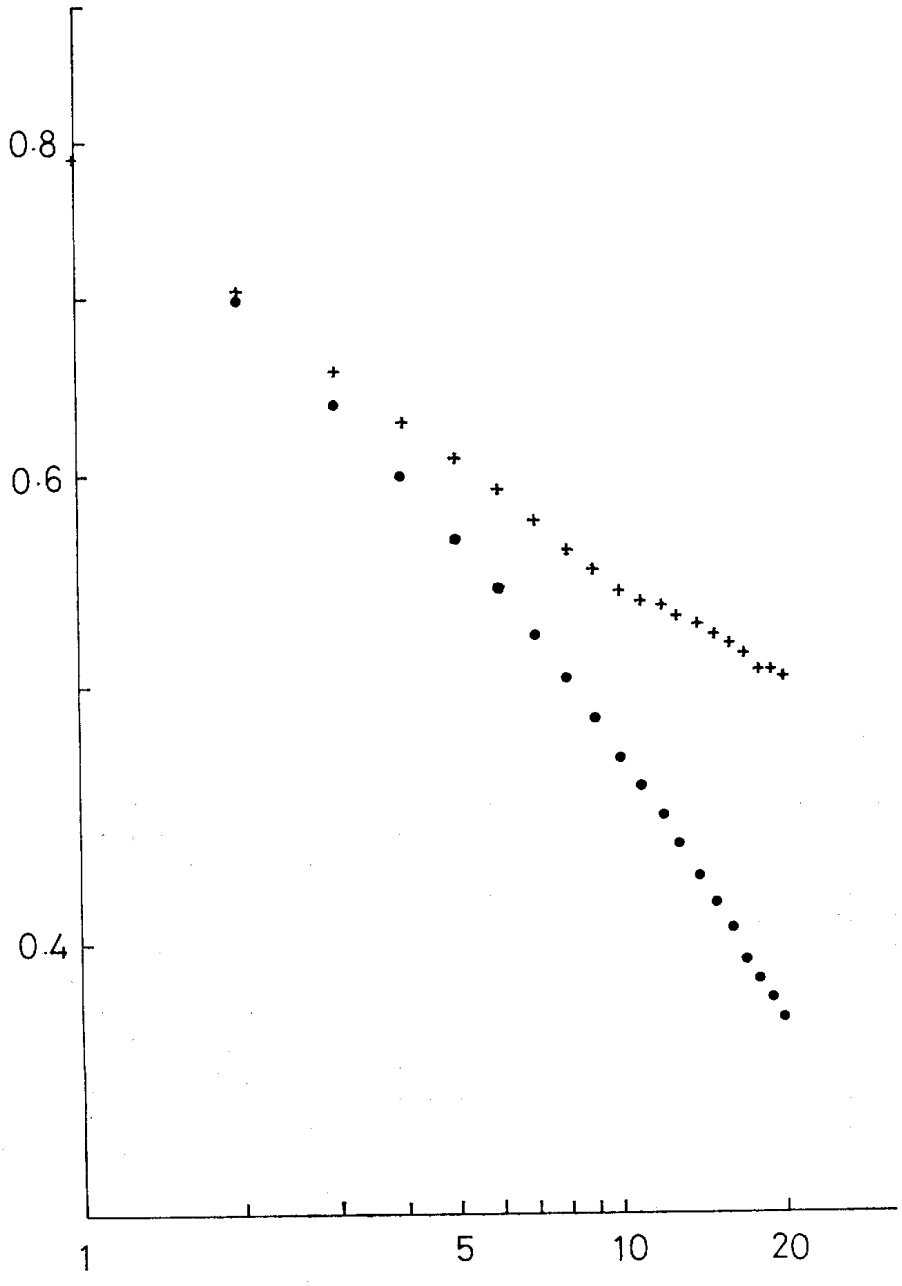

Fig. 6 The correlation function in a logarithmic scale at $T=0.4$, which are depicted against logarithmic lattice distance.

The non-linear σ model is a continuous-space limit of the classical Heisenberg model. An instanton solution of the σ model with topological charge n has the form

$$w=\frac{\prod_{i=1}^{n}\sigma(z-a_i)}{\prod_{i=1}^{n}\sigma(z-b_i)}, \tag{4.3}$$

where σ is a Sigma-function with quasi-periodicity on the complex plane [27] and z is a complex co-ordinate of position. The σ field variable $(\sigma_x,\ \sigma_y,\ \sigma_y)$ is connected to the complex field w in the following manner;

$$w=\frac{\sigma_x+i\sigma_y}{1+\sigma_z}, \tag{4.4}$$

The parameters a_i and b_i are the positions of instantons and anti-instantons, respectively. As follows from the form (4.3),

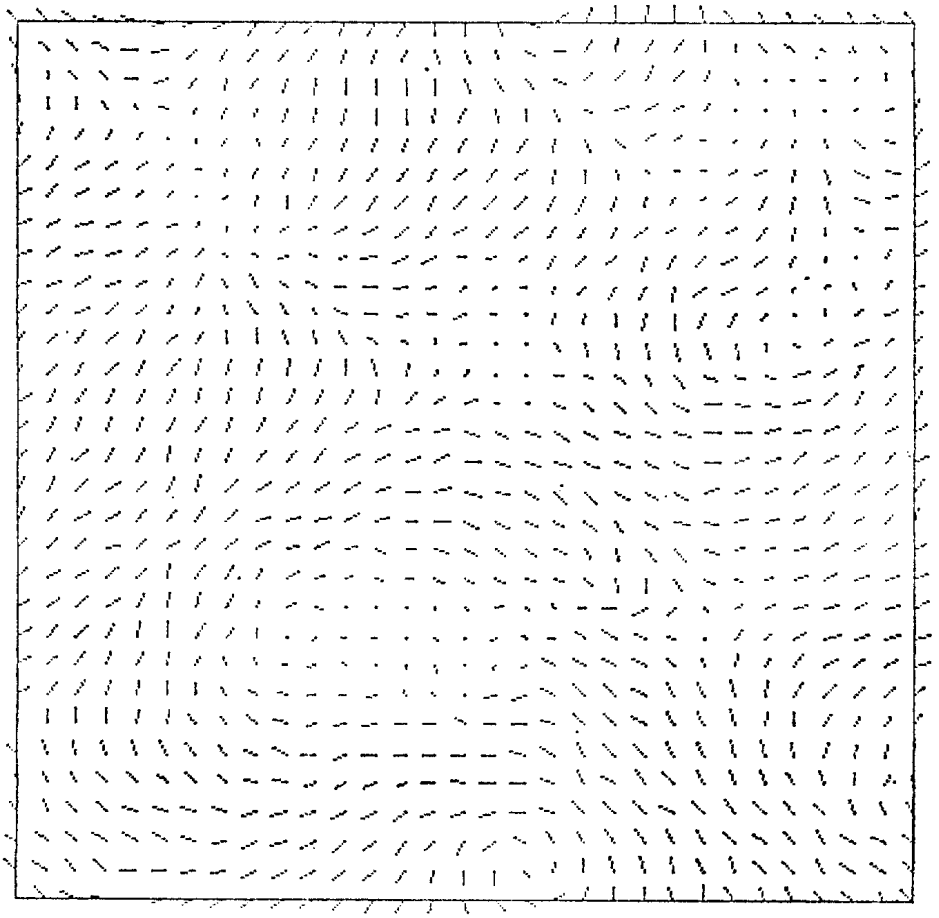

Fig. 7a The projection of spins onto the lattice plane on a 31×31 lattice in the thermal equilibrium at $T=0.2$. The updating method is (H1).

we find vortices, sources and sinks in fig. 7a, if we regard a spin vector projected onto the lattice plane as a velocity vector of a "fluid". Figure 7b shows a spin cofiguration at $T=0.2$. We have examined the transformation of the spin configuration in the thermal equilibrium at various temperatures. No abrupt change of the configuration can be found in the crossover region.

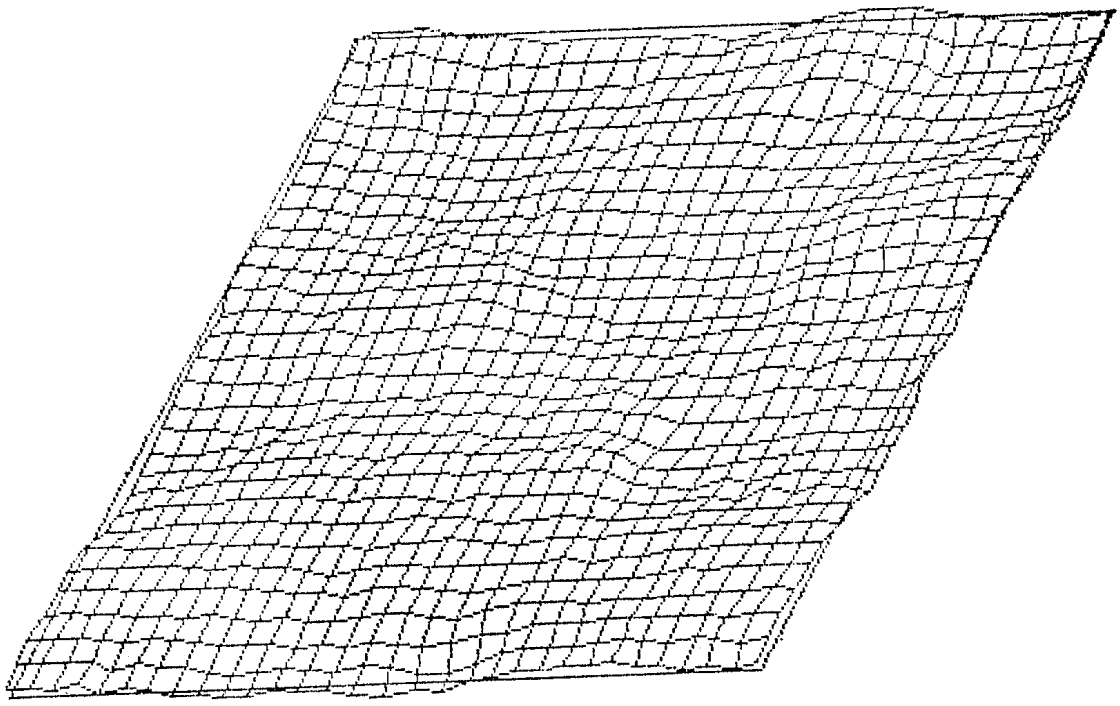

Fig. 7b Spin configuration at the same condition as fig. 7a. The tips of spins are connected by the lines for the guide of eyes.

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